Elasticity of smectic liquid crystals with in-plane orientational order and dispiration asymmetry

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The Nelson-Peliti formulation of the elasticity theory of isolated fluid membranes with orientational order emphasizes the interplay between geometry, topology, and thermal fluctuations. Fluid layers of lamellar liquid crystals such as smectic-C, hexatic smectics, and smectic-C^* are endowed with in-plane orientational order. We extend the Nelson-Peliti formulation so as to bring these smectics within its ambit. Using the elasticity theory of smectics-C^*, we show that positive and negative dispirations (topological defects in Smectic-C^* liquid crystals) with strengths of equal magnitude have disparate energies—a result that is amenable to experimental tests.

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I. INTRODUCTION

Smectic liquid crystals (smectics) are one-dimensional "solids" composed of two-dimensional fluid layers. Thermotropic [1] as well as lyotropic [2] smectics having orientational order in the fluid layers (in-plane orientational order) exhibit a rich profusion of symmetries. As a consequence, smectics display a wide variety of topological defects [1,3–5], such as dislocations, disclinations, and dispirations, including a range of curvature defects known as focal conics [3,5]. For example, smectic-C (SmC) has in-plane vectorial order, and supports dislocations as well as disclinations. Smectic-C^* (SmC^*) is chiral, has vectorial order, and supports exotic topological defects called dispirations.

Motivated by the discovery of liquid crystalline smectic $L_{\beta'}$ phase of phospholipid membranes with vectorial in-plane order [6], and the feasibility of obtaining almost isolated, deformable membranes by hyperswelling it [7], Nelson and Peliti [8] formulated the elasticity theory of isolated fluid membranes with in-plane orientational order. This elegant formulation brings out the interplay between elasticity, topological defects, and thermal fluctuations in isolated fluid membranes endowed with in-plane orientational order. It establishes that Gaussian curvature of a membrane is apt to act as a source of disclinations in the orientational order. Conversely, disclinations tend to bend flat, deformable membranes [9]. These reciprocal effects help to mitigate the overall stress from bending of membranes, and that from deformations in the orientational order. Positive and negative disclinations of equal strength prefer locally positive (sphere-like) and negative (saddle-like) Gaussian curvatures, respectively, leading to asymmetry in their energies [9–11]. Disclination induced buckling of nematic, and smectic vesicles has been observed experimentally [12].

As is the case for membranes, smectic layers bend because of thermal fluctuations and in response to externally applied stresses. The physics that describes the interplay between elasticity, topological defects, and thermal fluctuations as brought out by the Nelson-Peliti formulation is, therefore, applicable to smectics—one-dimensional, periodic stacks of orientationally ordered, two-dimensional fluid membranes.

In this paper we adapt and extend the Nelson-Peliti formulation [8] to smectics with in-plane orientational order and develop the continuum elasticity of such smectics. It is applicable to all smectics, and multilamellar, lyotropic vesicles, which have in-plane orientational order (excepting smectics such as very short pitched chiral SmC^*, which are not suited to a continuum description). Using our results for the elasticity theory of SmC^*, we investigate the structure and energetics of dispirations in SmC^* and show that dispirations with a negative index have a lower energy (per unit length) as compared to those with a positive index of the same strength. This result illustrates that the generalization mentioned above can lead to new, experimentally testable consequences in the mature field of smectic liquid crystals. Throughout this paper we assume that smectic as well as orientational order is well established; the treatment of phase transitions such as nematic-SmA-SmC [13] and the effect of thermal fluctuations [9,10] is outside the scope of this paper.

This paper is organized as follows. In Sec. II we present a brief review of the Nelson-Peliti formulation of the elasticity theory of isolated membranes endowed with orientational order. In Sec. III we discuss the elasticity theory of achiral as well as chiral smectics with in-plane orientational order. The structure and energetics of dispirations in smectics-C^* are discussed in Sec. IV.

II. THE NELSON-PELITI FORMULATION

In this section we give a brief account of the Nelson-Peliti formulation of elasticity of fluid membranes with in-plane orientational order and the corresponding equations of equilibrium. The well-known Helfrich free energy [14] of an up-down symmetric, deformable fluid membrane (regardless of orientational order) is

$$F_{\mathrm{H}} = \int \left[\frac{\kappa}{2} H^2 + \kappa_{\mathrm{G}} K \right] dS, \tag{2.1}$$

where H is the mean curvature, K is the Gaussian curvature, κ and κ_{G} are elastic constants, and the integral is over the surface of the deformed membrane surface. Gaussian curvature K is a total divergence and does not contribute to the equations of equilibrium (the Euler-Lagrange equations). In the Monge

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gauge, the membrane surface is described by using the height function $h = h(x,y)$ in the Cartesian coordinate system. In this gauge the lowest order, approximate expressions for H and K are

$$H \simeq \nabla_\perp^2 h, \quad \text{and}$$
$$K \simeq \left(\partial_x^2 h\right)\left(\partial_y^2 h\right) - (\partial_x\partial_y h)(\partial_y\partial_x h), \tag{2.2}$$

where $\nabla_\perp^2 = \partial_x^2 + \partial_y^2$ is the two-dimensional Laplacian operator. Within this approximation the surface integral in Eq. (2.1) is over $dS \simeq dx\,dy$ rather than over the deformed membrane surface. The Helfrich free energy refers only to deformations of the shape of the membrane and not to the deformation of the orientational order embedded in it.

Before discussing the elastic free energy for orientationally ordered membranes, we consider the simplest continuum model with orientational order, the continuum xy model, which has the low-temperature elastic free energy [4],

$$F_{xy} = \frac{k_s}{2}\int (\nabla\theta)^2 dx dy, \tag{2.3}$$

where k_s is the spin-wave stiffness, the unit xy-spin vector $\hat{\boldsymbol{m}} = (\cos\theta, \sin\theta)$, and $\boldsymbol{\nabla} = (\partial_x, \partial_y)$ is the gradient operator. We wish to generalize the flat-space xy model described above to spins on a deformable surface.

On curved membranes orientational order gets frustrated, as evidenced by the familiar fact that a hairy ball cannot be combed flat without creating disclinations of total index 2. On curved surfaces, ordinary derivatives of vector fields have to be replaced by covariant derivatives. The generalization of Eq. (2.3) to spins on a deformable surface involves defining the appropriate "covariant derivative of θ" on a curved membrane. For deformable membranes the square-gradient elastic free energy Eq. (2.3) takes the form [8]

$$F_\theta = \frac{K_A}{2}\int (\boldsymbol{\nabla}\theta - \boldsymbol{A})^2 dS, \tag{2.4}$$

where the "vector potential" $\boldsymbol{A}$ is a local gauge field that corrects $\boldsymbol{\nabla}\theta$ so as to compensate for membrane curvature, and the integral is over the deformed membrane surface. $\boldsymbol{A}$ is called the spin connection. To the lowest order the components of $\boldsymbol{A}$ are given by

$$A_i = \tfrac{1}{2}\,\epsilon_{jk}\,\partial_k[(\partial_i h)(\partial_j h)] \tag{2.5}$$

in the Monge gauge, where ϵ_{ij} is the totally antisymmetric unit symbol with $\epsilon_{xy} = -\epsilon_{yx} = 1$, and repeated indices are summed over. Thus, F_θ necessarily involves a coupling between θ and h fields.

The geometry of the membrane (represented by the Gaussian curvature K) and the topology of the θ field on it (represented by the disclination density $\mathscr{S}$, see below) are connected through [8]

$$\boldsymbol{\nabla}\times\boldsymbol{\nabla}\theta = \mathscr{S}\,\hat{\boldsymbol{n}}, \quad \text{and}$$
$$\boldsymbol{\nabla}\times\boldsymbol{A} = K\,\hat{\boldsymbol{n}}, \tag{2.6}$$

where $\hat{\boldsymbol{n}}$ is the unit normal to the membrane. The disclination density (see Sec. IV A for a simple introduction to disclinations),

$$\mathscr{S}(\boldsymbol{x}) = 2\pi\sum_m q_m\,\delta^{(2)}(\boldsymbol{x} - \boldsymbol{x}_m), \tag{2.7}$$

with discrete disclination charges q_m located at $\boldsymbol{x}_m$. The importance of the relation Eqs. (2.6) is brought out by the compatibility condition discussed below.

Minimization of F_θ with respect to the θ field gives the equation of equilibrium [9],

$$\frac{\delta F_\theta}{\delta\theta} = -K_A\,\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\theta - \boldsymbol{A}) = 0. \tag{2.8}$$

The Airy stress function χ, defined by

$$\partial_i\theta = \epsilon_{ij}\partial_j\chi, \tag{2.9}$$

identically satisfies $\delta F_\theta/\delta\theta = 0$. However, χ has to obey the condition

$$\nabla^2\chi = \mathscr{S} - K, \tag{2.10}$$

which ensures compatibility between the shape of the membrane and topology of the orientational order embedded in it.

Minimization of the total elastic free energy $F_H + F_\theta$ with respect to the height-field h in the Monge gauge yields the approximate "nonlinear, hexatic von Kármán shape equation" of [9]

$$\frac{\kappa}{K_A}\nabla^4 h = \left(\partial_y^2\chi\right)\left(\partial_x^2 h\right) + \left(\partial_x^2\chi\right)\left(\partial_y^2 h\right) - 2(\partial_x\partial_y\chi)(\partial_x\partial_y h). \tag{2.11}$$

The compatibility condition Eq. (2.10) and the shape Eq. (2.11) form the pair of coupled, nonlinear partial differential equations of bulk equilibrium.

III. ELASTICITY OF SMECTICS

This section is organized as follows. In Sec. III A we briefly discuss the elasticity theory of SmA. This is followed by the simplest, isotropic elasticity theories of SmC, smectics with hexatic order (SmF, SmI, SmL), and SmC^* in Sec. III B, where the shape-orientational order coupling via the spin-connection term is emphasized.

A. Smectic-A liquid crystals

Before addressing the extension of the spin-connection formulation to smectics with orientational order, we briefly review the standard elasticity theory of SmA [4,5]. SmA does not have in-plane orientational order (Fig. 1). However, the layer compression and layer bend terms introduced below are common to all smectics, regardless of the presence of in-plane orientational order. In the ground state, flat, fluid layers of thermotropic SmA, typically composed of rod-like molecules, form a periodic stack along the layer normal, which we take to be along the z axis. The Frank director $\boldsymbol{n}_F$ is also oriented along the layer normal. The elastic free energy of SmA is a functional of the displacement field $u(x,y,z)$, which, in the continuum, describes the displacement of the layers along the z axis. The elastic free energy of SmA is [4,5]

$$F_{Sm}[u] = \int\left[\frac{B}{2}(\partial_z u)^2 + \frac{K}{2}(\nabla_\perp^2 u)^2 + K_G\tilde{K}\right]dV, \tag{3.1}$$

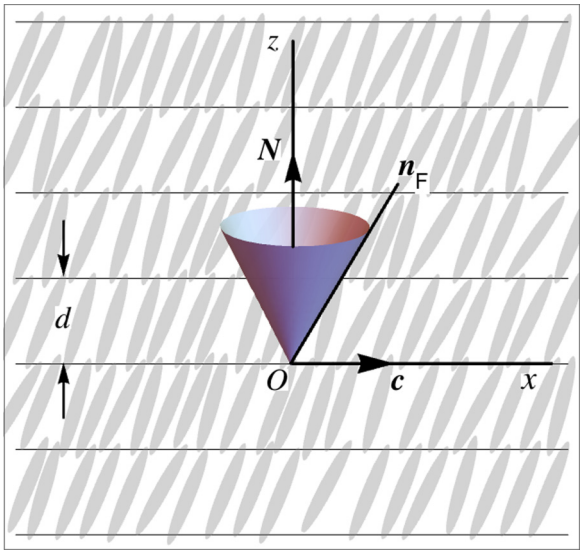


FIG. 1. Schematic of smectics: $\boldsymbol{n}_F \equiv -\boldsymbol{n}_F$ is the unit, apolar Frank director that specifies the average orientation of molecules; $\boldsymbol{N}$ is the unit layer normal. The equilibrium layer spacing is d. In SmA $\boldsymbol{n}_F \parallel \boldsymbol{N}$; Sm$A$ does not have in-plane orientational order, the molecular orientation is not tilted. In SmC, the projection of $\boldsymbol{n}_F$ onto the layer plane, the polar vector $\boldsymbol{c}$, spontaneously breaks the continuous azimuthal symmetry. The plane spanned by $\boldsymbol{n}_F$ and $\boldsymbol{N}$ (the xz plane) is a mirror plane with a point of inversion. SmC^* has a chiral structure, in which the mirror symmetry of SmC is lost; $\boldsymbol{c} = c\,(\cos(q^*z), \sin(q^*z), 0)$ in the ground state, i.e., $\boldsymbol{n}_F$ lies on a cone with its tip on a helix with pitch $P^* = 2\pi/q^*$.

where $\nabla_\perp^2$ is the two-dimensional Laplacian operator, and dV is the volume element. The first term on the right-hand side of Eq. (3.1) describes the free-energy cost for layer compression. We note that the layer-compression term (having coefficient B) is not rotationally invariant. In the Eulerian picture of elasticity theory the rotationally invariant nonlinear elasticity for layer compression is obtained by the replacement $\partial_z u \to \partial_z u - (1/2)(\boldsymbol{\nabla} u)^2$ in Eq. (3.1) above [4]. The terms with coefficients K and K_G give the free-energy costs for the mean and the Gaussian curvatures of the layers, respectively. The two-dimensional, flat-space Laplacian of the displacement, $\nabla_\perp^2 u(x,y,z)$, is an approximation to $(1/2)\tilde{H}(x,y,z)$, where $\tilde{H}(x,y,z)$ is the "mean curvature" at a point in the three-dimensional smectic. The expression

$$\tilde{K}(x,y,z) = \left(\partial_x^2 u\right)\left(\partial_y^2 u\right) - (\partial_x\partial_y u)(\partial_y\partial_x u) \tag{3.2}$$

for the "Gaussian curvature" at a point is valid to the same order of approximation as $2\tilde{H}(x,y,z) \simeq \nabla_\perp^2 u$. Gaussian curvature is a total divergence, integrates to the boundary surface, and does not contribute to the bulk energy. In writing Eq. (3.1) it is implicitly assumed that the local Frank director $\hat{\boldsymbol{n}}_F$ is "tied" or locked to the local layer normal $\hat{\boldsymbol{N}}$, so that $\hat{\boldsymbol{n}}_F \parallel \hat{\boldsymbol{N}}$ even in the deformed configuration. The elastic free-energy Eq. (3.1) for smectic layer distortions (compression and bend) used in this paper is the continuum, Landau-Peierls version, which is valid for "type-I" smectics (those for which the Ginzburg parameter $\kappa = \lambda_p/\xi < 1/\sqrt{2}$, where λ_p denotes twist penetration depth, and ξ is the smectic correlation length) [4].

B. Smectics with in-plane orientational order

In this section we first consider SmC (Fig. 1), the simplest lamellar liquid crystal with vectorial in-plane order. Next, we consider smectics with in plane nematic and hexatic order, followed by chiral SmC^* (Fig. 1). Although the elasticity theory of smectics with in-plane order discussed here is not fully covariant, it captures the essential physics of the crucial coupling between shape and orientational order. The derivation of its covariant version will be discussed elsewhere.

1. *Smectic-C liquid crystals*

In the undeformed, ground state of SmC, the three-dimensional, unit Frank director $\hat{\boldsymbol{n}}_{F0}$ can be written in terms of its projection $\boldsymbol{c}_0$,

$$\hat{\boldsymbol{n}}_{F0} = \left(\boldsymbol{c}_0, \sqrt{1 - c_0^2}\right), \tag{3.3}$$

where the two-dimensional vector $\boldsymbol{c}_0$ has the components $\boldsymbol{c}_0(x,y,z) = c_0\,(\cos\psi_0(x,y,z),\ \sin\psi_0(x,y,z))$ in the xy plane, and $c_0 = \sin A_0$, where A_0 is the angle between the Frank director and the local layer normal (the half-apex angle of the cone in Fig. 1). As in the elasticity of SmA, we assume that the tilt-angle A_0 of the molecular director is locked, so that the magnitude c_0 is fixed. Thus, the projection of the Frank director in the deformed state of SmC is described by $\boldsymbol{c}(x,y,z) = c_0\,(\cos\psi(x,y,z),\ \sin\psi(x,y,z))$. The elastic variables for SmC are then the displacement field u of the layers, and the azimuthal angle ψ of the Frank director. The angle ψ is analogous to the angle θ used for membranes in Sec. II. To the lowest order the elastic free energy of SmC is given by

$$F_C[u,\psi] = F_{Sm}[u] + \int f_\psi\, dV, \tag{3.4}$$

where we have used the elastic free energy for layer distortions $F_{Sm}[u]$ is given by Eq. (3.1), and f_ψ is the elastic free-energy density for deformations in the ψ field (see below). The orientational order, described by ψ, is inevitably coupled to the shape of smectic layering. In a general deformation, smectic layering can bend and acquire Gaussian curvature. The arguments of Sec. II that lead to the introduction of spin-connection in defining the proper gradient of θ also hold for ψ. The angle ψ can have spatial variations within the plane of a given layer, as well as across the layering. Therefore, the lowest-order (in-plane) isotropic elastic free-energy density for SmC has to be of the form

$$f_\psi = \frac{\tilde{K}_A}{2}\,(\boldsymbol{\nabla}_\perp\psi - \tilde{\boldsymbol{A}}_\perp)^2 + \frac{K_N}{2}\,(\partial_z\psi)^2, \tag{3.5}$$

where $\psi = \psi(x,y,z)$. The first, and the second terms on the right-hand side are the elastic free-energy density costs for in-plane deformations and deformations across the layering, respectively. The term with the coefficient $\tilde{K}_A$ describes the crucial shape-orientational order coupling. The approximate expression for the spin-connection is

$$\tilde{A}_{\perp i}\,(x,y,z) = \epsilon_{jk}\,\partial_k\,[(\partial_i u)\,(\partial_j u)], \tag{3.6}$$

where it is important to note that i,j,k run over x,y, and that $u = u(x,y,z)$. It is easy to check that the Gaussian curvature $\tilde{K} = (\boldsymbol{\nabla}_\perp \times \tilde{\boldsymbol{A}}_\perp)\cdot\boldsymbol{N}$, where the layer normal $\boldsymbol{N} \simeq (-\partial_x u, -\partial_y u, 1)$.

The elastic coefficients $\tilde{K}_A$ and K_N have the dimensions of force. A straightforward comparison of the Frank free-energy density for nematics with Eq. (3.5) above gives a rough estimate of $\tilde{K}_A$, and K_N in terms of the Frank elastic coefficients K_1 (splay), K_2 (twist), and K_3 (bend) [15]. The elastic coefficient $\tilde{K}_A$ involves splay as well as bend in the $\boldsymbol{c}$- field, which in turn involves all three Frank elastic coefficients. In the one constant approximation ($K_1 = K_2 = K_3 = \mathcal{K}$), and for small tilt angles A_0, $\tilde{K}_A \simeq \mathcal{K} A_0^2$. The coefficient $K_N \simeq K_2 \sin^4 A_0 + K_3 \sin^2 A_0 \cos^2 A_0$ includes twist and bend deformations in the Frank director. Both $\tilde{K}_A$ and K_N vanish ($A_0 = 0$) in the SmA phase.

2. Other smectics

The elasticity theory Eq. (3.4) of SmC is easily modified to describe that of other smectics. For example, the lowest order, isotropic elastic free-energy of a smectic with nematic in-plane order is obtained by merely redefining ψ as the angle of deviation of the nematic director from its orientation in the undeformed state. For thermotropic, hexatic SmB that does not have tilt-order [16,17], the elastic free energy is obtained by redefining the hexatic bond-orientational order ψ modulo $2\pi/6$. Thermotropic, achiral hexatic smectics such as SmI and SmF have two kinds of in-plane orientational order, one from the tilt orientation and one from the hexatic order. The tilt orientation in SmI is toward the hexatic bond, whereas that for SmF is midway between the hexatic bond angles [18]. Hexatic SmL has tilt orientation between 0 and $\pi/6$ and is, therefore, chiral [19]. The elastic free-energy Eq. (3.4) can be easily extended to SmL by introducing two angles, ψ and φ, corresponding to the tilt and hexatic orders, respectively, and by including known symmetry-allowed elastic couplings between these fields [17]. There are lyotropic smectics that appear to possess the same symmetries as SmI, SmF, and SmL (named $L_{\beta \mathrm{I}}$, $L_{\beta \mathrm{F}}$, and $L_{\beta \mathrm{L}}$, respectively) [19]; however, their structures have not yet been characterized unambiguously [20].

3. Smectic-C* liquid crystals

As indicated in Fig. 1, SmC^* is chiral, with vectorial order in the plane of smectic layers. In the undeformed state, SmC^* has uniform pitch along the layer normal. The lowest order, harmonic elasticity of SmC^* is given by replacing f_ψ of Eq. (3.4) by

$$f_{\psi *} = \frac{\tilde{K}_A}{2}(\boldsymbol{\nabla}_\perp \psi - \tilde{\boldsymbol{A}}_\perp)^2 + \frac{K_N}{2}(\partial_z \psi)^2 - h^* \partial_z \psi, \qquad (3.7)$$

where the first two terms on the right-hand side are the same as those of f_ψ for SmC Eq. (3.5), and we have introduced a new term with the pseudoscalar coefficient h^* describing the chiral strength, which reflects the chirality of SmC^*. The angle ψ is a pseudoscalar, therefore $h^* \partial_z \psi$ is a true scalar, as it should be. This term ensures that the undeformed, ground-state structure of SmC^* is chiral, with a uniform pitch $P^* = 2\pi K_N / h^*$, and penalizes deviations of ψ away from it. There is no symmetry-allowed, harmonic elastic coupling between the compression $\partial_z u$ and gradients of ψ. We note that the continuum elasticity theory described above holds for SmC^* with $|P^*| \gg d$. In Sec. IV below, we use the elasticity theory of SmC^* developed above to establish the asymmetry in dispiration energies.

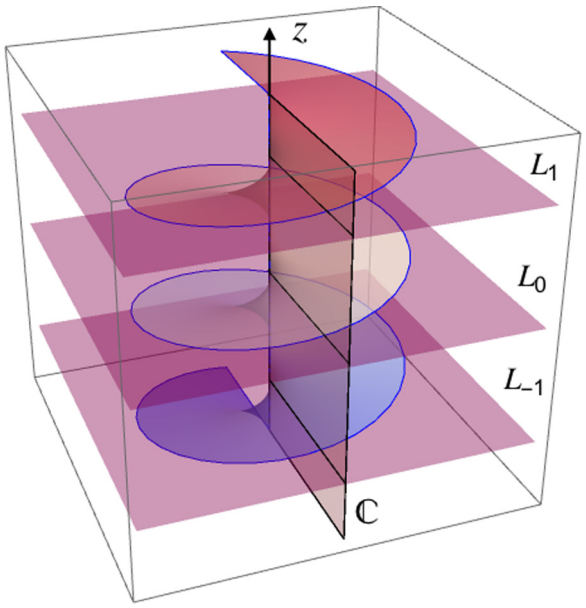


FIG. 2. The planar surface L_i labels the ith smectic layer in the reference lattice of SmA, with interlayer spacing d. Making a vertical cut $\mathbb{C}$ (shaded rectangle) through the layers, identifying the left lip of the cut on L_{i-1} to the right lip of the cut on L_i, and letting the system relax leads to the right-handed, half-helicoidal surface shown. This is the Volterra construction of a screw dislocation. The z axis is the singular dislocation line, and $\boldsymbol{b} = d\,\hat{\boldsymbol{z}}$ is the Burgers vector.

IV. DISPIRATIONS IN Sm-C^*

Owing to their periodicity, smectics with orientational order support dislocations as well as disclinations. Dispirations are topological line defects in SmC^*. Dispirations have a mixed character; their structure involves features of both dislocations and disclinations. Before discussing wedge-screw dispirations in SmC^*, we review the structure and energetics of screw dislocations and disclinations (Sec. IV A). This is followed by the characterization of the structure of dispirations (Sec. IV B) and their energetics (Sec. IV C).

A. Screw dislocations and disclinations

As mentioned in the Introduction, smectics with in-plane orientational order support dislocations as well as disclinations. In this section we give a brief pedagogical review of these line defects.

1. Screw dislocations in SmA

A screw dislocation line in SmA (Fig. 2) is characterized by the topological condition

$$\oint du = \oint \boldsymbol{\nabla} u \cdot d\boldsymbol{l} = nd = b, \qquad (4.1)$$

where the integral is over any closed loop around the dislocation line, n is an integer, d is the smectic layer spacing, and b is the magnitude of the Burgers vector. The Burgers vector $\boldsymbol{b}$ of a screw dislocation is defined in relation to the direction of the screw dislocation line $\hat{\boldsymbol{\lambda}}$ by using the right-hand rule for traversing the closed loop. $\hat{\boldsymbol{\lambda}}$ can be freely chosen to be along either $\hat{\boldsymbol{z}}$ or $-\hat{\boldsymbol{z}}$, since the ground state of SmA is invariant

under the transformation $z \to -z$. If the displacement b of Eq. (4.1) is parallel to $\hat{\boldsymbol{\lambda}}$, then $\boldsymbol{b} = +b\,\hat{\boldsymbol{z}}$. If the displacement b is antiparallel to $\hat{\boldsymbol{\lambda}}$, then $\boldsymbol{b} = -b\,\hat{\boldsymbol{z}}$ [4]. Thus, right-handed screw dislocations have $\boldsymbol{b} = b\,\hat{\boldsymbol{z}}$, whereas left-handed screw dislocations have $\boldsymbol{b} = -b\,\hat{\boldsymbol{z}}$.

The solution of the equation of equilibrium,

$$-B\,\partial_z^2 u + K\,\nabla_\perp^4 u = 0, \tag{4.2}$$

corresponding to the elastic free energy Eq. (3.1), satisfying the topological condition Eq. (4.1) with $b = d$ is

$$u(x,y,z) = \frac{d}{2\pi}\arctan\frac{y}{x}, \tag{4.3}$$

The function $\arctan(y/x)$ is just the polar angle in cylindrical polar coordinates, and the solution Eq. (4.3) describes a half-helicoid (Fig. 2). This surface is a minimal surface (has zero mean curvature; $\nabla_\perp^2 u = 0$). It is locally saddle-like, and therefore has negative Gaussian curvature. The half-helicoid has a singular line running along the z axis. Surrounding the singular line, strains are of order unity in a region having a size of order d. This region, where the smectic ordering gets destroyed, is called the core of the dislocation. Substituting Eq. (4.3) into Eq. (3.1), we find that within the linear elasticity theory used here, the elastic free energy of a screw dislocation is zero; the only contribution to the free energy of a screw dislocation in SmA is that from the destruction of smectic order at the core [5].

We note that the solution Eq. (4.3) has been obtained by assuming harmonic elasticity for layer compression. As stated in Sec. III A, the harmonic elasticity is not rotationally invariant. An exact solution for the displacement field of *edge dislocations* in SmA has been obtained in Ref. [21] using the nonlinear, rotationally invariant expression for layer-compression elasticity (see Sec. III A), albeit with the approximate, linear expression for the mean curvature of smectic layering. This solution fits well to experimentally studied displacement field profiles of edge dislocations in cholesteric fingerprint textures [22]. To our knowledge the exact solution to the full nonlinear problem has not yet been obtained for a screw dislocation in SmA. In this paper we do not address the energetics of dislocation cores (elastic strain is of order unity near the cores), which is outside the purview of elasticity theory.

The Volterra construction for a screw dislocation in SmA is shown in Fig. 2. The same construction can be carried out for a screw dislocation in SmC, without any discontinuity in the $\boldsymbol{c}$ field across the cut plane. However, carrying out the Volterra construction of a screw dislocation in SmC^* results in a discontinuity in the $\boldsymbol{c}$ field across the cut plane; ψ has a discontinuity of $d_0/|P^*|$ across each joint. We return to this issue in Sec. IV B.

2. *Disclinations—xy model*

An isolated, single disclination in the xy model is a point vortex characterized by the topological condition

$$\oint d\theta = \oint \nabla\theta \cdot d\boldsymbol{l} = 2\pi s, \tag{4.4}$$

where the integral is along any closed loop enclosing the singular disclination point, and s is called the disclination index. For the xy model, s has to be an integer, whereas for a two-dimensional nematic s can take values that are integer multiples of $1/2$ [4]. For a distribution of discrete disclinations Eq. (4.4) above can be written as

$$\epsilon_{ij}\,\partial_i\partial_j\theta(\boldsymbol{x}) = \mathscr{S}(\boldsymbol{x}), \tag{4.5}$$

where we have used Stokes's theorem, and where the disclination density $\mathscr{S}(\boldsymbol{x}) = 2\pi\sum_m q_m\,\delta^{(2)}(\boldsymbol{x} - \boldsymbol{x}_m)$, with discrete disclination charges q_m located at $\boldsymbol{x}_m$.

The solution to the equation of equilibrium,

$$-k_s\,\nabla^2\theta = 0, \tag{4.6}$$

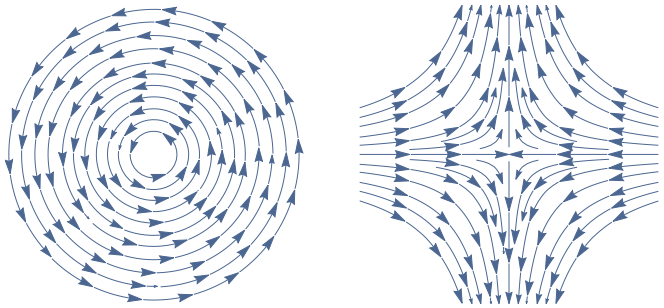
corresponding to the elastic free energy Eq. (2.3), which satisfies the topological condition Eq. (4.4) is

$$\theta = s\arctan(y/x). \tag{4.7}$$

Thus, the simplest $+1$ disclinations have either radial or circular streamlines centered at the disclination point, whereas the simplest -1 disclinations have a hyperbolic texture of streamlines (Fig. 3). Substituting Eq. (4.7) into (2.3), we find that the energy of a disclination is

$$E_s = 2\pi k_s\,s^2\ln(R/\xi) + E_c, \tag{4.8}$$

where R is the system size, ξ is the small-length cutoff for the disclination core, and E_c accounts for the free-energy cost from the destruction of xy order in the core.



(a) (b)

FIG. 3. Elliptic $(+1)$ and hyperbolic (-1) disclinations in the xy model. Upon traversing an anticlockwise, closed circuit, the vector field rotates in anticlockwise sense through 2π for a $+1$ disclination and in clockwise sense through 2π for a -1 disclination.

In fluid membranes with hexatic order, disclinations with the smallest strength have indices $\pm 1/6$. A fivefold disclination can be obtained by removing a wedge of angle $2\pi/6$ in the bond order, thus leaving fivefold bond order at the disclination point. A fivefold disclination has the index $+1/6$. A sevenfold disclination is obtained by adding a wedge of angle $2\pi/6$ in the bond order, and has the index $-1/6$. As stated in the Introduction, disclinations can buckle membranes provided κ/K_A is sufficiently small, thus leading to asymmetry in the energies of disclinations having indices of the same magnitude but opposite signs [9,10].

Disclinations in smectics are line defects rather than point defects. In smectics with in-plane nematic order, s can have half-integer values, since $\hat{\boldsymbol{n}}_F \equiv -\hat{\boldsymbol{n}}_F$. In Sm$C$, disclinations have integer indices because $\boldsymbol{c}$ is a polar vector.

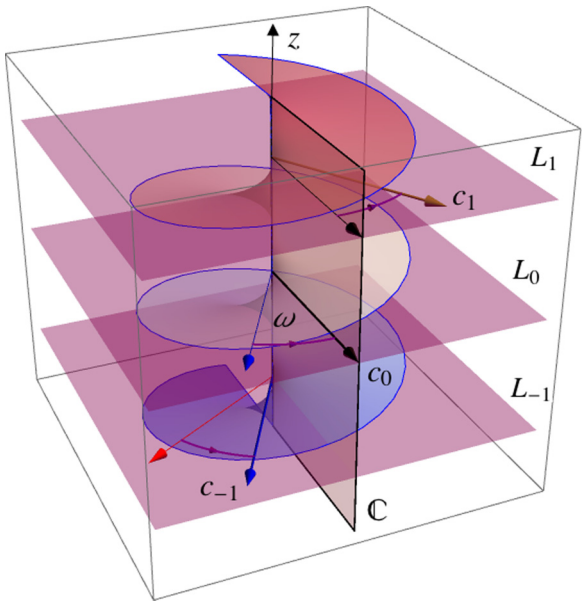


FIG. 4. Volterra construction for a dispiration in SmC^*: L_i (light planar surfaces) and $\boldsymbol{c}_i = c_0(\cos\psi_i, \sin\psi_i)$ (thick arrows) represent the ith smectic layer and the corresponding $\boldsymbol{c}$ field with pitch P^*. In the laboratory frame, $\boldsymbol{c}_0 \parallel \hat{\boldsymbol{x}}$. Thin arrows on L_i represent $\boldsymbol{c}_{i-1}$. Making a vertical cut $\mathbb{C}$ (shaded rectangle) through the layers and identifying the left lip of the cut on L_{i-1} to the right lip of the cut on L_i leads to a mismatch in the $\boldsymbol{c}$ field across $\mathbb{C}$. *To eliminate the mismatch, wedges of angle $\omega = d/|P^*|$ in the $\boldsymbol{c}$ field need to be inserted at the central singular line—one wedge of angle ω per layer*. Each wedge is a negative, *partial disclination*, since it does not correspond to a symmetry operation of the ground state of SmC^*. Post-relaxation, the construction described above leads to a wedge-screw dispiration—a screw dislocation associated with partial disclinations in each smectic layer.

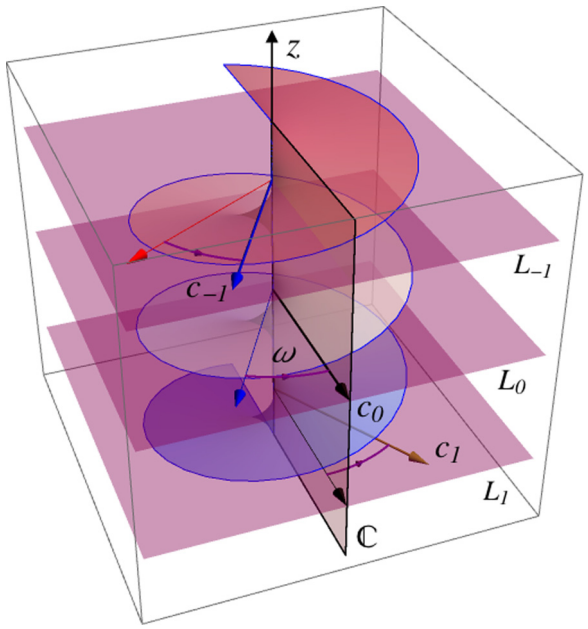


FIG. 5. A dispiration with $\mathtt{s}_d > 0$. As in Fig. 4, the screw dislocation is right-handed; $\boldsymbol{b} = d\,\hat{\boldsymbol{z}}$. However, the chirality of SmC^* is opposite of that shown in Fig. 4; $\hat{\boldsymbol{\lambda}} = -\hat{\boldsymbol{z}}$. Note that eliminating the mismatch in the $\hat{\boldsymbol{c}}$ field requires *removal* of wedges of angle ω.

B. Characterization of dispirations

The caption of Fig. 1 has a description of the structure of SmC^*. The Volterra construction of a screw dislocation in SmC^* leads to frustration in the vector order (Fig. 4) that can be healed by introducing *partial* disclinations. This combination of a screw dislocation and partial disclinations is called a wedge-screw dispiration [23–25]. Using simple polarizing microscopy, dispirations have been observed in antiferroelectric SmC^* [1,26]. In what follows, we focus on the characterization of dispirations.

Because of the chirality of SmC^*, dispiration lines can be assigned an unambiguous orientation. This is not the case for screw dislocation lines in achiral smectics such as SmA or SmC. SmC^* has no mirror plane. In particular, the xy plane is not a mirror plane. The direction of the dispiration line $\hat{\boldsymbol{\lambda}}$ can be fixed by exploiting the inherent chirality of the $\hat{\boldsymbol{c}}$ field in the ground state of SmC^* as follows. First, we label smectic layers by integers i such that the ψ field, *as defined in the reference, right-handed cylindrical polar coordinate system*, satisfies $\psi_{i+1} - \psi_i = \omega = d/|P^*| > 0$ (see Fig. 4). Next, we orient the dispiration line along a unit vector $\hat{\boldsymbol{\lambda}}$ that is in the direction of increasing i. In Fig. 4, $\hat{\boldsymbol{\lambda}} \parallel \hat{\boldsymbol{z}}$. To find the Burgers vector $\boldsymbol{b}$ we traverse an oriented circuit around $\hat{\boldsymbol{\lambda}}$ using the right-hand rule, as in Sec. IV A. The screw-dislocation component of the dispiration shown in Fig. 4 has $\boldsymbol{b} = +d\,\hat{\boldsymbol{z}}$ (the screw dislocation is right-handed). The partial-disclination component of the dispiration of Fig. 4 is negative (see Sec. IV A).

We define the index of a wedge-screw dispiration as $\mathtt{s}_d = -\omega = -(\hat{\boldsymbol{\lambda}} \cdot \boldsymbol{b})/|P^*|$; the dispiration shown in Fig. 4 has $\mathtt{s}_d < 0$, whereas the one shown in Fig. 5 has $\mathtt{s}_d > 0$. The dispiration index $\mathtt{s}_d$ captures the chirality of SmC^* (the direction of $\hat{\boldsymbol{\lambda}}$), as well as the handedness of the screw dislocation (the direction of $\boldsymbol{b}$). The minus sign in the definition of $\mathtt{s}_d$ is chosen to ensure that it matches the sign of the partial disclinations associated with the screw dislocation.

C. Energetics of dispirations

The elastic free energy of dispirations has been calculated in Ref. [25] using the results of Ref. [27] for the displacement field u of a screw dislocation in SmC. The "flat-space" elastic free-energy density of SmC^* in Ref. [25] does not use the spin-connection coupling. The stability conditions for the elastic energy used in Ref. [27] result in misleading solutions for the displacement field for screw dislocations in both SmC and SmC^* [28]. For a $\boldsymbol{c}$ field of fixed magnitude, the appropriate solution for screw dislocations is a simple half-helicoid, within the approximations used in our calculations below. As in SmA, the screw dislocation component of dispirations costs only core energy.

We now calculate the dispiration energy per unit length. In cylindrical polar coordinates, the compatibility condition Eq. (2.10) and the height Eq. (2.11) lead to the simple solution $\psi = \omega\phi$. The elastic free energy is $F_{\psi*} = \int f_{\psi*} dV$, where $f_{\psi*}$ is given by Eq. (3.7). In cylindrical polar coordinates (ρ,ϕ,z), $dV = \rho d\rho d\phi dz$. However, for a screw dislocation (half-helicoid of pitch b) parametrized by the position vector $\boldsymbol{R} = (\rho\cos\phi, \rho\sin\phi, [d/(2\pi)]\phi)$, $\rho > 0$, the appropriate vol-

ume element is $dV = \sqrt{\rho^2 + [d/(2\pi)]^2} d\rho d\phi dz$ (the surface area of a half-helicoid over one pitch is larger than that of a circular disk). We have checked that $\psi = \omega\phi$ remains a solution in the helicoidal coordinate system, in which $(A_\rho, A_\phi) = (0, -\rho/\sqrt{\rho^2 + [d/(2\pi)]^2})$. Compensating for the components $A_\rho = 0$, $A_\phi = -1$ for the planar reference state of smectic layers [9] and using the volume element that is appropriate to the half-helicoidal shape, we find that the energy per unit length of a straight wedge-screw dispiration, written in terms of ω, is

$$\frac{E}{\pi K_A} \simeq \omega^2 (c_1 + \ln \lambda_2) + \omega [c_2 + 2 \ln(\lambda_1/\lambda_2)] + E_c + c_3, \tag{4.9}$$

where $\lambda_2 = (\lambda + \lambda_1)$, $\lambda_1 = \sqrt{1 + \lambda^2}$, and $\lambda = L/d$ (not to be confused with the unit vector $\hat{\boldsymbol{\lambda}}$ along the dispiration line) for a system of size L. E_c is the energy cost for destruction of smectic order in the dispiration core. In Eq. (4.9), $c_1 = -\ln(1 + \sqrt{2}) \simeq -0.88$, $c_2 = \ln(1/2) + 2\ln(1 + \sqrt{2}) \simeq 1.07$, and $c_3 \simeq 0.02$ is very weakly dependent on λ. As in the case of SmA, the screw dislocation component does not contribute to the total elastic energy within the approximations used. The "flat-space" result of Ref. [25] does not have the crucial term linear in ω [see Eq. (4.9)] that leads to dispiration asymmetry. From Eq. (4.9), $E(\omega) < E(-\omega)$. For $\lambda \gg 1$, $E(\omega) - E(-\omega) \simeq -2K_A \omega < 0$. Recalling that the twist angle ψ between adjacent smectic layers $\omega = -\mathrm{s}_d$, we find that SmC^* liquid crystals prefer dispirations with negative s_d—a result that is amenable to experimental tests. The dispiration of Fig. 4 has a lower energy per unit length than that of Fig. 5. The Gaussian curvature of the screw dislocation is negative, and negative Gaussian curvature acts as a source of negative disclinations. Thus, our result for the energetics of dispirations is consistent with those of Refs. [9,10] for disclinations in membranes.

Some remarks of particular relevance to our result on dispiration asymmetry are in order. Within the SmC^* phase, the pitch P^* is known to change considerably with temperature. Moreover, this dependence is nonmonotonic [29]. Elaborate phenomenological theories [30,31] have been proposed to explain the observed variation of the SmC^* pitch with temperature. Based upon the discussion in Sec. III B we expect $K_A \simeq 3 \times 10^{-7}$ dyne within the SmC^* phase. Our result $E(\omega) - E(-\omega) \simeq -2K_A \omega$ implies that the smaller the pitch, the larger the magnitude of disclination asymmetry. Based partially upon the analysis of Refs. [9,10], and on the experimental demonstration of disclination induced buckling in nematic and smectic vesicles [12], we believe that our result on asymmetry in dispiration energies in SmC^* is qualitatively robust, and would persist in a more detailed, fully covariant version of the elasticity theory of smectics with in-plane orientational order.

V. SUMMARY

We have extended the Nelson-Peliti formulation of the elasticity theory of orientationally ordered membranes to thermotropic, as well as lyotropic smectic liquid crystals. It leads to asymmetry in the energies of positive and negative dispirations. This result demonstrates that our adaption of the Nelson-Peliti formulation is capable of leading to qualitatively new results in the field of lamellar liquid crystals with in-plane orientational order.

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